1,4-Dioxane, 2-ethyl-5-methyl-

Other names: 2-Ethyl-5-methyl-1,4-dioxane
Inchi: InChI=1S/C7H14O2/c1-3-7-5-8-6(2)4-9-7/h6-7H,3-5H2,1-2H3
InchiKey: DPXGZEPGOMVZDJ-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCC1COC(C)CO1
Mol. weight [g/mol]: 130.18
CAS: 53907-91-8

Physical Properties

Property code	Value	Unit	Source
gf	-147.44	kJ/mol	Joback Method
hf	-417.83	kJ/mol	Joback Method
hfus	22.75	kJ/mol	Joback Method
hvap	40.32	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.200		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	913.00		NIST Webbook
tb	428.34	K	Joback Method
tc	630.96	K	Joback Method
tf	224.93	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.11	J/mol×K	428.34	Joback Method
cpg	305.59	J/mol×K	597.19	Joback Method
cpg	292.65	J/mol×K	563.42	Joback Method
cpg	279.04	J/mol×K	529.65	Joback Method
cpg	264.75	J/mol×K	495.88	Joback Method
cpg	249.78	J/mol×K	462.11	Joback Method
cpg	317.87	J/mol×K	630.96	Joback Method

dvisc	0.0003579	Pa×s	428.34	Joback Method
dvisc	0.0004645	Pa×s	394.44	Joback Method
dvisc	0.0006333	Pa×s	360.54	Joback Method
dvisc	0.0009207	Pa×s	326.63	Joback Method
dvisc	0.0014597	Pa×s	292.73	Joback Method
dvisc	0.0026113	Pa×s	258.83	Joback Method
dvisc	0.0055665	Pa×s	224.93	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53907918&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume